

Large nucleation distances from impurities in the cosmological quark-hadron transition

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Abstract

We calculate the mean nucleation distance, d_{nuc} , in a first order cosmological quark-hadron phase transition. For homogeneous nucleation we find that self-consistent inclusion of curvature energy reduces d_{nuc} to $\lesssim 2\text{cm}$. However, impurities can lead to heterogeneous nucleation with d_{nuc} of several meters, a value high enough to change the outcome of Big Bang nucleosynthesis.

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I. INTRODUCTION

A number of authors [1–4] have suggested that inhomogeneities in the baryon number density were produced in the cosmological quark-hadron phase transition and perhaps even persisted to the time of nucleosynthesis, which could alter the abundances of light elements. For this to happen, a few criteria have to be met, though. First of all, only a first order quark-hadron transition seems capable of generating large baryon number fluctuations. Whether the transition is first order is still an unsettled question (see e.g. Ref. [5]). Secondly, the mean distance between high and low baryon density regions, denoted l , has to be larger than approximately one meter comoving at $T = 100\text{MeV}$ [4], if inhomogeneous nucleosynthesis results are to differ from the standard homogeneous nucleosynthesis results (otherwise, neutron and proton diffusion will erase the inhomogeneities prior to nucleosynthesis). Other important parameters are the average density contrast between high and low-density regions, the average volume fraction of high-density regions, and the baryon to photon ratio.

We assume that the transition is first order and focus in this paper on determination of the most important of the parameters, the mean distance l .

A first order quark-hadron transition in the expanding Universe can in general terms be described as follows. As the color deconfined quark-gluon plasma cools below the critical temperature, $T_c \approx 100\text{MeV}$, it becomes energetically favorable to form color confined hadrons (primarily pions and a tiny amount of neutrons and protons due to the conserved net baryon number). However, the new phase does not show up immediately. As is characteristic for a first order phase transition, some supercooling is needed to overcome the energy expense of forming the surface of bubbles of the new hadron phase. When a hadron bubble is nucleated, latent heat is released, and a spherical shock wave expands into the surrounding supercooled quark-gluon plasma. This reheats the plasma to the critical temperature, preventing further nucleation in a region passed by one or more shock fronts [6] (for the range of parameters used in the present investigation, bubble growth is described by deflagrations, where a shock front precedes the actual phase transition front. However, if the shock fronts are very weak the quark-gluon plasma may not be reheated enough to sufficiently prevent new bubble nucleations in such regions [6]. This reduces the mean distance. We will neglect this possibility, because of the very small amounts of supercooling we deal with here). The nucleation stops when the whole Universe has reheated to T_c . This part of the phase transition passes very fast, in about $0.05\mu\text{s}$, during which the cosmic expansion is totally negligible. After that, the hadron bubbles grow at the expense of the quark phase and eventually percolate or coalesce; almost in equilibrium at T_c . The transition ends when all quark-gluon matter has been converted to hadrons, neglecting possible quark nugget production [1].

How much the system has to supercool before the first hadron bubbles show up determines the distance between nucleation sites. This distance is called the (comoving) mean nucleation distance, d_{nuc} . It is also roughly the distance between the shrinking, high-baryon-density quark droplets. l is half that distance, and when we take into account that the Universe expanded about 50% during the phase transition, we have

$$l \simeq 0.8 \left(\frac{T_c}{100\text{MeV}} \right) d_{nuc}, \quad (1)$$

where the factor $T_c/100\text{MeV}$ scales the value of d_{nuc} from a given critical temperature to $T = 100\text{MeV}$, where l is defined.

In the bag model we can approximate d_{nuc} in homogeneous nucleation theory without curvature energy in terms of the bag constant, B , by

$$d_{nuc} \approx 13 \left(\frac{145\text{MeV}}{B^{1/4}} \right)^2 \left(\frac{4B}{L} \right) \left(\frac{\sigma}{0.035B^{3/4}} \right)^{3/2} \text{ cm}, \quad (2)$$

where L is the latent heat and σ the surface tension. Lattice QCD calculations [7] suggest that $\sigma \lesssim 0.24T_c^3$, Ref. [8] finds $\sigma \simeq 0.025T_c^3$ and $L \simeq 0.4B$. With $T_c \simeq 0.68B^{1/4}$, this gives $d_{nuc} \simeq 0.1\text{m}$ for $T_c > 100\text{MeV}$.

We calculate the surface tension self-consistently within the multiple reflection expansion framework of the MIT bag model and get $\sigma \lesssim 0.035B^{3/4}$ and $L \simeq 4B$, corresponding to $d_{nuc} \lesssim 0.1\text{m}$. But we also self-consistently take into account the important curvature term and find a crude approximate formula for d_{nuc} ,

$$d_{nuc} \approx 1.8 \left(\frac{145\text{MeV}}{B^{1/4}} \right)^2 \left(\frac{4B}{L} \right) \text{ cm}. \quad (3)$$

Note, that in this approximation the mean nucleation distance depends only on the bag constant (or T_c). Thus the overall effect of including a curvature term is roughly a factor of 7 reduction of d_{nuc} . With these estimates of d_{nuc} in mind it hardly seems possible to get any significant deviations from standard nucleosynthesis, if homogeneous nucleation theory applies.

However, homogeneous nucleation may not be the prime mechanism responsible for hadron formation. It is well-known from every day life that first order transitions are normally facilitated by impurities, such as dust or ions and container walls. Think e.g. of a charged particle entering a cloud chamber, or boiling water where (half) bubbles are formed at the bottom of the pot. Such nucleations are denoted heterogeneous. Thus it is obvious to consider the effect of such impurities on the quark-hadron phase transition. Candidates are the topological impurities, like primordial black holes, magnetic monopoles, and cosmic strings or relic fluctuations from the electroweak transition.

The idea that impurities could play a role in the cosmological quark-hadron transition is not new (see e.g. [9] for a general discussion of the role of impurities in cosmological phase transitions), but normally it has been argued [3] that the presence of impurities would just act as extra seeds for nucleation sites together with the homogeneous nucleation sites and thus reducing d_{nuc} .

As demonstrated below, this picture is not necessarily correct—there are circumstances where impurities lead to a dramatic *increase* in d_{nuc} , maybe even to a value of several meters, resurrecting inhomogeneous Big Bang nucleosynthesis. We find that three limits with, respectively, small, medium and huge amounts of impurities, compared to the number of homogeneous nucleation sites, have to be considered. Certainly, if only very few impurities are present in the early Universe d_{nuc} will be determined solely by homogeneous nucleation. In the other extreme, for a huge number of impurities, they will determine a d_{nuc} smaller than the one obtained from homogeneous nucleation. So neither of these cases give large mean nucleation distances.

Any impurity tends to lower the cost in energy when creating the surface of the new phase. Therefore bubbles of the new phase will nucleate easier around an impurity at a

smaller amount of supercooling. This means that shock spheres from nucleations around impurities start reheating the Universe earlier. And for some impurity number densities the whole Universe has already been reheated before the amount of supercooling has increased to a value where homogeneous nucleation sets in. In this case d_{nuc} depends on the impurity number density, n , on the time when heterogeneous nucleation starts, and on the time when homogeneous nucleation becomes important. For a large range of parameters, d_{nuc} can be very big.

We will make this qualitative discussion much more quantitative in Section III, where we also present a self-consistent bag model calculation of homogeneous nucleation, including for the first time the important curvature terms. In Sec. II we describe the thermodynamics of the phase transition and the multiple reflection expansion of the MIT bag model, which we use to calculate the thermodynamical quantities. Section IV contains a general discussion and a summary of our results.

II. THERMODYNAMICS AND THE BAG MODEL

All the necessary thermodynamical information about the two phases is contained in the thermodynamical potential $\Omega(T, \mu, V, S, C)$. μ is the chemical potential, V the volume, and finite size corrections enter via the surface area, S , and the extrinsic curvature, C .

$$\Omega = -T \ln Z, \quad (4)$$

where Z is the grand partition function. All other thermodynamical quantities can be derived from Ω . For instance, the bulk pressure P is

$$P = - \left(\frac{\partial \Omega}{\partial V} \right)_{T, \mu, S, C}, \quad (5)$$

and the surface tension σ

$$\sigma = \left(\frac{\partial \Omega}{\partial S} \right)_{T, \mu, V, C}. \quad (6)$$

Because of the huge photon to baryon ratio, we can neglect all chemical potentials and simplify the equations for Ω when we want to calculate d_{nuc} , since $(\mu/T) \sim 10^{-9}$ in the early Universe (see e.g. [10]). (This is not true if one is interested in following the further evolution of baryon density contrasts.)

A. The quark phase

The quark phase consists of massless gluons, massless (or with masses of 5–10 MeV) u and d quarks, and a massive s quark, where we use a broad interval, $m_s/\text{MeV} \in [50, 300]$. In most calculations we have integrated numerically the s -quark distribution function; however for simplicity we neglect the small s -quark contribution to the cosmic density when calculating the cosmological time-temperature relation from the Friedmann equations. The gluons contribute with 16 degrees of freedom, while each of the quarks has 12 degrees of freedom

(including antiparticles). In thermal equilibrium with both phases during the transition are (statistical weight in parenthesis) electrons(4), muons(4), neutrinos(6) and photons(2). The contributions from these particles cancel when we study pressure differences.

The behavior of quarks is mainly governed by the strong interaction. It can, at least in principle, be described in the QCD model. But since QCD is a non-perturbative theory at low energy and therefore *very* difficult to handle, phenomenological models, like the MIT bag model, or lattice QCD calculations are used in practice. The basic idea of the bag model is that the quarks can be treated as an (almost) ideal gas confined to a finite region of space, a bag, by what we may think of as an external pressure, B , called the bag constant. In the multiple reflection expansion framework [11] a statistical approach is taken and finite size effects of the bag are explicitly incorporated in the density of states formula Eq. (10) in terms of geometrical factors.

What value to take for the phenomenological bag constant is at present very uncertain; it could even be temperature dependent. A lower limit on the bag constant of $(145\text{MeV})^4$ is set by the stability of nuclei, especially ^{56}Fe , relative to ud -quark matter. There is no upper limit available from physical considerations. Lattice QCD calculations typically favor $B^{1/4}$ above 200MeV. We use here a broad interval for the bag constant, $B^{1/4}/\text{MeV} \in [145; 245]$. It was shown, in the $T = 0$ limit, by Farhi and Jaffe [12] that a QCD coupling constant different from zero can largely be absorbed in a reduction of the bag constant. We assume this is valid at finite temperatures too and put $\alpha_s = 0$.

The multiple reflection expansion was originally derived for a quark droplet embedded in a hadron gas. But Mardor and Svetitsky [13] have shown that it can also be used to describe a hadron bubble in a quark plasma, provided the signs of the volume and curvature terms are changed. The formulae below are for a quark droplet. The thermodynamical potential of the quark phase is then given by

$$\Omega_q = \sum_i \Omega_i + BV, \quad (7)$$

where Ω_i is the thermodynamical potential for a single fermion (quark) or boson (gluon), given as

$$\Omega_i = -T \ln Z_i. \quad (8)$$

Here Z_i is the corresponding grand partition function

$$\ln Z_i = \pm \int_0^\infty dk \rho(k) \ln \left(1 \pm e^{-\sqrt{k^2+m_i^2}/T} \right) \quad (9)$$

(upper sign for fermions, lower for bosons) where the density of states is obtained from the multiple reflection expansion

$$\begin{aligned} \rho(k) = g \left\{ \frac{k^2 V}{2\pi^2} + f_S \left(\frac{k}{m} \right) k \oint_S dS \right. \\ \left. + f_C \left(\frac{k}{m} \right) \oint_S \left(\frac{1}{R_1} + \frac{1}{R_2} \right) dS + \dots \right\}, \end{aligned} \quad (10)$$

g is the statistical weight of the particle. The volume term is universal and we recognize the finite size effects from the surface area, S , in the second term, and from the extrinsic

curvature, C , in the third term. Higher order terms are neglected. Assuming that the quark droplets are spherical, then $V = 4\pi R^3/3$, $S = 4\pi R^2$ and $C = 8\pi R$. The coefficient functions $f_J(k/m)$ are for quarks [14]

$$f_S\left(\frac{k}{m}\right) = -\frac{1}{8\pi} \left[1 - \frac{2}{\pi} \arctan \frac{k}{m}\right], \quad \lim_{m \rightarrow 0} f_S = 0 \quad (11)$$

and

$$f_C\left(\frac{k}{m}\right) = \frac{1}{12\pi^2} \left[1 - \frac{3}{2} \frac{k}{m} \left(\frac{\pi}{2} - \arctan \frac{k}{m}\right)\right],$$

$$\lim_{m \rightarrow 0} f_C = -\frac{1}{24\pi^2} \quad (12)$$

f_C has not been calculated from the multiple reflection expansion for massive quarks, but Eq. (12) gives a perfect fit to shell model calculations for strangelets [15]. For the massless gluons we have [13]

$$f_S = 0, \quad f_C = -\frac{1}{6\pi^2}. \quad (13)$$

Note, that these results for gluons have been confirmed by pure glue QCD lattice calculations [16].

B. The hadron phase

We treat the hadron phase as an ideal pion gas, where we calculate the pressure from Ω_i using Eq. (8) for bosons and only including the volume term in the density of states formula Eq. (10). This approximation is justified because the pions, with masses around the critical temperature 100-200MeV, are the lightest hadrons and semi-relativistic while all other hadrons are nonrelativistic and therefore contribute negligibly to the pressure for $T \lesssim 200\text{MeV}$. The pion pressure is much smaller than the bag pressure so even the pressure from fully relativistic pions will only increase the critical temperature one percent. A perhaps more serious problem is that pions are not “point-like” particles and excluded volume effects should be taken into account. The pions could in principle contribute to the surface term (and curvature term as well), we do not know. However, the pions have only 3 degrees of freedom, while each of the quarks have 12, so we would expect only minor corrections.

C. Hadron bubbles in quark-gluon plasma

The change in the thermodynamical potential, when a quark matter droplet of radius R_q is formed in a hadron gas, is

$$\Delta\Omega_{q\text{-droplet}} = P_h V_q + \Omega_q(R_q). \quad (14)$$

Because the photon-lepton gas is in thermal equilibrium with both phases, it does not contribute to $\Delta\Omega$. Only in pressure ratios is it of importance to include the photon-lepton

contribution. In the cosmological quark-hadron phase transition hadron bubbles are formed from a quark-gluon plasma. Mardor and Svetitsky [13] have shown that this situation can be described simply by inverting the system, i.e let $R_q \rightarrow -R_h$. This inversion affects only the signs of the volume and curvature terms and not the absolute value of any of the coefficients. $\Delta\Omega$ can then be written as

$$\Delta\Omega_{h\text{-bubble}} = -P_h V_h + \Omega_q(-R_h). \quad (15)$$

or

$$\Delta\Omega = -\frac{4\pi}{3}\Delta P R^3 + 4\pi\sigma R^2 - 8\pi\gamma R, \quad (16)$$

where we have suppressed the index h on the hadron bubble radius. If we relate the temperature and bag constant as

$$T \equiv xB^{1/4}, \quad T_c \equiv x_c B^{1/4}, \quad (17)$$

then from the multiple reflection expansion we have

$$\Delta P \equiv P_h - P_q = P_\pi + B - P_s - \frac{37}{90}\pi^2 x^4 B, \quad (18)$$

where the pion pressure is (we treat the three pion types alike and use a mean mass of $m_\pi = 138\text{MeV}$)

$$P_\pi = -\frac{3x}{2\pi^2}B \int_0^\infty du u^2 \ln \left(1 - e^{-\sqrt{u^2 + \tilde{c}^2}/x}\right), \quad \tilde{c} = \frac{m_\pi}{B^{1/4}} \quad (19)$$

and the s quark pressure

$$P_s = \frac{6x}{\pi^2}B \int_0^\infty du u^2 \ln \left(1 + e^{-\sqrt{u^2 + \tilde{c}^2}/x}\right), \quad \tilde{c} = \frac{m_s}{B^{1/4}}. \quad (20)$$

The critical temperature is found from $\Delta P = 0$ (the corresponding x_c lies between 0.67 and 0.70). The surface tension, where only the massive s quarks contribute, is given by

$$\sigma = \sigma_s = \frac{3x}{2\pi}B^{3/4} \int_0^\infty du u \left(1 - \frac{2}{\pi} \arctan \frac{u}{\tilde{c}}\right) \times \ln \left(1 + e^{-\sqrt{u^2 + \tilde{c}^2}/x}\right). \quad (21)$$

And finally the curvature coefficient

$$\gamma = \frac{19}{36}x^2 B^{1/2} + \gamma_s, \quad (22)$$

where

$$\gamma_s = -\frac{x}{\pi^2}B^{1/2} \int_0^\infty du \left[1 - \frac{3}{2}\frac{u}{\tilde{c}} \left(\frac{\pi}{2} - \arctan \frac{u}{\tilde{c}}\right)\right] \times \ln \left(1 + e^{-\sqrt{u^2 + \tilde{c}^2}/x}\right). \quad (23)$$

γ is always larger than zero because of the large positive contribution from the gluons, even though γ_s can be negative depending on the mass of the s quark. So the curvature energy is always negative when making a hadron bubble.

The latent heat per volume, released in a first order transition, is defined as

$$L \equiv -T_c \left[\frac{\partial \Delta P}{\partial T} \right]_{T_c}. \quad (24)$$

Eq. (18) can easily be differentiated with respect to temperature and the latent heat calculated numerically for fixed bag constant and strange quark mass. In Fig. 1 we have plotted the latent heat as a function of the strange quark mass. And we show the effect of including higher mesonic states up to 1 GeV (the higher mesonic states have much less influence on the critical temperature, because the bag constant contributes with about 95% of the pressure needed to maintain pressure equilibrium between the two phases. That is why we can safely disregard heavier mesons for $T_c \leq 200\text{MeV}$). It is evident that these states only have a minor influence on the latent heat. A good approximation is to use

$$L \simeq 4B \quad (25)$$

independent of m_s . We adopt this approximation, but notice that some lattice QCD calculations suggest [8] that the latent heat is much smaller, $L \simeq 0.4B$. We will discuss the possible discrepancy later.

III. NUCLEATION THEORY

In classical nucleation theory the nucleation rate (number of nucleations per volume per time) is given by [17,18]

$$p(T) = C(T) \exp\left(-\frac{\Delta F_c}{T}\right), \quad (26)$$

where ΔF_c is the minimum work needed to create the smallest possible growing bubble, equal to the change in Helmholtz free energy, and $\exp(-\Delta F_c/T)$ is the probability of making a growing bubble. The pre-exponential factor depends in detail on the model by which the bubble growth is described. Csernai and Kapusta [19] have calculated $C(T)$ in the cosmological case (relativistic particles and almost zero baryon number), but without a curvature term, and get

$$C(T) = \frac{16}{3^{5/2}\pi} \frac{\sigma^{5/2}\lambda^3}{\xi_q^4 L^2 T^{3/2}} R_c, \quad (27)$$

where R_c is the radius of a critical size bubble and $\xi_q \approx 0.7\text{fm}$ is the surface thickness of the bubble. ξ_q has to be much smaller than R_c , which it is since $R_c \approx 50\text{fm}$, typically. Finally the shear viscosity λ is approximated by

$$\lambda \simeq \frac{1.12}{\alpha_s^2 \ln \alpha_s^{-1}} T^3, \quad (28)$$

where α_s is the strong coupling constant. Fortunately, as we will show, a temperature dependent pre-exponential factor like Eq. (27) is not important when we want to determine d_{nuc} . Thus, the often used dimensional estimate $C(T) \approx T_c^4$ is sufficient for this purpose.

A. Homogeneous Nucleation

This subsection is for a major part a straight forward generalization of the work done by Fuller, Mathews and Alcock [3] to take a varying pre-exponential factor and, more important, a curvature term into account. Their results (with the correction mentioned in [20]) are recovered in the limit of constant pre-exponential factor and vanishing curvature.

The change in Helmholtz free energy is equal to the change in the thermodynamical potential in the limit of vanishing chemical potentials. Thus,

$$\Delta F(R, T) = -\frac{4\pi}{3}\Delta P R^3 + 4\pi\sigma R^2 - 8\pi\gamma R. \quad (29)$$

The radius of a critical size bubble is found by putting $\partial\Delta F/\partial R$ equal to zero. From this equation we get two critical radii

$$R_{\pm} = \frac{\sigma}{\Delta P} \left(1 \pm \sqrt{1 - \frac{2\Delta P\gamma}{\sigma^2}} \right). \quad (30)$$

The smaller radius corresponds to a local minimum in the free energy (see Fig. 2), the larger to a local maximum. As pointed out in [13] this local minimum has some serious consequences, if it is real and not just a shortcoming of the multiple reflection expansion of the bag model, since it means that small hadron bubbles show up even above the critical temperature. It has been argued that these hadron bubbles are unstable [21], but at present it is unclear how to handle them. We will for now neglect this complication, keeping it in mind for later discussion.

A linear expansion of ΔP about the critical temperature gives

$$\Delta P = L\eta, \quad (31)$$

where L is the latent heat per volume, and the supercooling parameter for $T \leq T_c$ is

$$\eta \equiv \frac{T_c - T}{T_c}. \quad (32)$$

This expansion is valid for the small supercooling $\eta \ll 1$ we deal with in the cosmological quark-hadron transition. We then write $\Delta F_c = F(R_+, T) - F(0, T)$ as

$$\Delta F_c(\eta) = \frac{8\pi}{3} \frac{\sigma^3}{L^2\eta^2} \left(1 - \frac{3L\gamma}{\sigma^2}\eta + \left(1 - \frac{2L\gamma}{\sigma^2}\eta\right)^{3/2} \right). \quad (33)$$

Certainly ΔF_c can not be allowed to become negative if we insist on ignoring the minimum. This gives an upper limit on the supercooling parameter,

$$\eta \leq \frac{3}{8} \frac{\sigma^2}{L\gamma}. \quad (34)$$

Combining equations (26) and (33) gives the nucleation rate as a function of the small supercooling parameter, valid around the critical temperature:

$$p(\eta) = C(\eta) \exp \left[-\frac{8\pi}{3} \frac{\sigma^3}{L^2 T_c \eta^2} (1 - 3b\eta + (1 - 2b\eta)^{3/2}) \right] \quad (35)$$

where

$$b \equiv \frac{L\gamma}{\sigma^2}. \quad (36)$$

We see that $p(\eta)$ equals zero as we pass the critical temperature from above and increases very rapidly with η . As a result nearly all nucleation takes place at the lowest temperature, T_f , achieved during the supercooling phase. This means that we may generally approximate the pre-exponential factor with its value at T_f provided it is not *too* temperature dependent.

It turns out to be fruitful to make a linear expansion of $\ln p(\eta)$ about the time t_f corresponding to the temperature T_f

$$\ln p(t) \simeq \ln p(\eta_f) + \left[\frac{d \ln p}{d\eta} \right]_{\eta_f} \left[\frac{d\eta}{dT} \right]_{T_f} \left[\frac{dT}{dt} \right]_{t_f} (t - t_f), \quad (37)$$

or

$$p(t) \simeq p(\eta_f) \exp[-\alpha(t - t_f)]. \quad (38)$$

This is a good approximation because of the steepness of the nucleation rate (cf. Eq. (35)). We have implicitly assumed that the surface tension and curvature coefficient are independent of temperature. This is not true in the bag model. But there is nothing special at all about the critical temperature from the point of view of σ and γ . And since the amount of supercooling is very small we treat them as constants and use their values at T_c .

The temperature as a function of time is found by solving the Friedmann equations for a flat Universe consisting of a quark-gluon plasma, photons and leptons. It is, in the first order approximation we use, independent of the bag constant,

$$T \simeq \left(\frac{45}{16\pi^2 g_q G} \right)^{1/4} t^{-1/2}, \quad (39)$$

where G is the gravitational constant, and the statistical weight $g_q = 51.25$ (for simplicity we here neglect the small contribution from the semirelativistic s -quarks). α is then

$$\alpha = (41\pi G)^{1/2} \left(\frac{\pi}{3} T_c^2 \frac{C'(\eta_f)}{C(\eta)} + \frac{8\pi^2}{9} \frac{\sigma^3 T_c}{L^2 \eta_f^3} [2 - 3b\eta_f + (2 - b\eta_f)(1 - 2b\eta_f)^{1/2}] \right), \quad (40)$$

where $C' \equiv dC/d\eta$.

The mean nucleation distance is found from the total number density of nucleation sites

$$n_{nuc} \equiv d_{nuc}^{-3} = \int_{t_c}^{\infty} f(t) p(t) dt, \quad (41)$$

where $f(t)$ is the unaffected fraction of the Universe.

After a hadron bubble is nucleated a spherical shock front expands into the quark phase at a speed slightly above the sound speed, $v_s \simeq 3^{-1/2}$, and reheats it to the critical temperature, which prevents any further nucleation in a region crossed by one or more shock fronts [6]. We use the formula given by Guth and Tye [22] for the fraction of space not yet passed by one or more shock fronts (a slightly different approach can be found in [19]),

$$f(t) = \exp \left[- \int_{t_c}^t dt' f(t') p(T(t')) V(t', t) \right] \quad (42)$$

where t_c is the time corresponding to temperature T_c and $V(t', t)$ in this context is the reheated volume at time t caused by a bubble nucleated at time t' . $V(t', t)$ can be written as

$$V(t', t) \approx \frac{4\pi}{3} v_s^3 (t - t')^3. \quad (43)$$

For the short timescales involved here, we can safely neglect the cosmic expansion. This recursive formula for $f(t)$ can be simplified to a step function by a linear expansion, giving

$$f(t) \simeq \begin{cases} 1 - \frac{4\pi}{3} v_s^3 \int_{t_c}^t dt' p(T(t')) (t - t')^3 & t < t_f \\ 0 & t \geq t_f \end{cases}. \quad (44)$$

The time t_f corresponds to the maximum supercooling η_f , where we demand the whole Universe to be reheated. The approximation succeeds because of the very rapid rise of the nucleation rate. If we introduce the approximation for the nucleation rate, Eq. (38), the integral in Eq. (44) can be analytically evaluated and

$$f(t) \simeq \begin{cases} 1 - \frac{8\pi v_s^3}{\alpha^4} p(\eta_f) e^{-\alpha(t_f - t)} & t < t_f \\ 0 & t \geq t_f \end{cases} \quad (45)$$

where terms $\exp[-\alpha(t_f - t_c)]$ have been neglected compared to terms $\exp[-\alpha(t_f - t)]$, because of the steepness of $p(t)$. Demanding the whole Universe to have been reheated at t_f gives an equation for the maximum amount of supercooling achieved during the transition

$$\frac{8\pi v_s^3}{\alpha^4} p(\eta_f) = 1. \quad (46)$$

It has an approximate solution given by

$$\begin{aligned} \eta_f &\simeq \frac{0.4}{\sqrt{2}} \frac{\sigma^{3/2}}{LT_c^{1/2}} \sqrt{1 - 3b\eta_f + (1 - 2b\eta_f)^{3/2}} \\ &\simeq 0.48 \frac{\sigma^{3/2}}{LT_c^{1/2}} \sqrt{1 - 3b\eta_f}. \end{aligned} \quad (47)$$

A finite γ approximately halves the critical amount of supercooling, since it turns out that $b\eta_f \simeq \frac{1}{4}$. The behavior of η_f is shown in Fig. 3. Notice, that η_f scales with $1/L$.

The approximate solution in Eq. (47) ignored the details of the pre-exponential factor, C . To see that this is justified, neglect for a moment the curvature term. It is then easy to show that

$$\eta_f = 4.1 \frac{\sigma^{3/2}}{LT_c^{1/2}} \times \left[195 + \ln C - 4 \ln \left(\frac{32\pi\sigma^3 T_c}{3L^2\eta_f^3} + T_c^2 \frac{C'}{C} \right) \right]^{-1/2}, \quad (48)$$

with all dimensional quantities in MeV-units. For the $C(\eta)$ in Eq. (27) $C'/C = -1/\eta_f$. Because

$$\frac{32\pi\sigma^3 T_c}{3L^2\eta_f^3} \gg \frac{T_c^2}{\eta_f}, \quad (49)$$

when η_f is approximated by Eq. (47), we can safely ignore the C'/C term. Thus a pre-exponential factor of the form Eq. (27) does not significantly influence the maximum amount of supercooling neither directly, not even changes in C of several orders of magnitude, nor through its derivative. This result is independent of bag model parameters. The same qualitatively picture holds when the curvature term is included, if we do nothing but substitute Eq. (30) for R_c . Notice however, that this may not be valid since the pre-exponential factor is derived without taking a curvature term into account.

The mean nucleation distance is found by substituting Eqs. (44) and (38) into Eq. (41) and integrating,

$$d_{nuc} = (16\pi)^{1/3} \frac{v_s}{\alpha}, \quad (50)$$

where terms like $\exp[-\alpha(t_f - t_c)]$ have been neglected. It should be emphasized that this is also a general result independent of bag model parameters. Only α is model dependent. With α from Eq. (40), neglecting the C'/C term, d_{nuc} becomes

$$d_{nuc} \simeq 1.3 \times 10^9 \left[\frac{L^2}{\sigma^3 T_c} \text{MeV}^2 \right] \eta_f^3 \times \left[\frac{1}{4} \left(2 - 3b\eta_f + (2 - b\eta_f) \sqrt{1 - 2b\eta_f} \right) \right]^{-1} \text{cm}. \quad (51)$$

Eq. (2) is found by inserting the first approximation for η_f from Eq. (47) with $\gamma = 0$. For $\gamma \neq 0$ one finds in the same manner from the second approximation in Eq. (47)

$$d_{nuc} \approx 1.8 \left(\frac{145 \text{MeV}}{B^{1/4}} \right)^2 \left(\frac{4B}{L} \right) \left(\frac{\gamma}{0.24B^{1/2}} \right)^3 \text{cm}, \quad (52)$$

but γ is very insensitive to varying s quark mass because of the large contributions from the massless species. Thus the last term is always close to unity and we recover Eq. (3). Note, the mean nucleation distance is also inversely proportional to the latent heat.

In Figure 4 we have plotted the mean nucleation distance as a function of the strange quark mass for a small and a large bag constant with and without the curvature term. Curves for intermediate bag constants lie between those two curves. This has been done by solving Eq. (46) numerically and inserting in Eq. (50) for d_{nuc} . For comparison the two approximative solutions, Eqs. (2) and (3) have been plotted, too. If we look at Eq. (50) we see that for increasing α , i.e. decreasing amount of supercooling, then the mean nucleation

distance decreases. This is because a larger α means a more sudden nucleation and more bubbles are needed in order to reheat the whole Universe at η_f . Inclusion of a curvature term lowers the energy barrier and thereby the maximum amount of supercooling, resulting in roughly a factor of 7 reduction of d_{nuc} .

B. Heterogeneous Nucleation

In a first order phase transition the presence of impurities lowers the energy barrier and thereby reduces the maximum amount of supercooling achieved during the transition. We assume that a number density, n , of impurities were present in the Universe prior to the quark-hadron transition. Candidates could be primordial black holes, magnetic monopoles, cosmic strings, or relic fluctuations from the electroweak transition. Especially the latter candidate is interesting because the horizon distance at the time of the electroweak transition ~ 0.3 cm ($t \sim 10^{-11}$ s, $T \sim 100$ GeV) has expanded three orders of magnitude to ~ 3 meters at the time of the quark-hadron transition. Further we assume that nucleation around all impurities takes place at a time t_i , where $t_c \leq t_i < t_f$, and that the bubble expansion is similar to the homogeneous case.

The combined nucleation rate can then be written as a sum of the nucleation rate around impurities and the homogeneous nucleation rate,

$$p_{com}(t) = n\delta(t - t_i) + p(\eta_f)e^{-\alpha(t_f-t)}, \quad (53)$$

where δ is Dirac's delta function. The unaffected fraction of the Universe can still be evaluated in the same approximation leading to Eq. (45) although the approximation becomes slightly poorer.

$$f(t) \simeq \begin{cases} 1 - \frac{4\pi v_s^3}{3} \left(n(t - t_i)^3 + \frac{6}{\alpha^4} p(\eta_f) e^{-\alpha(t_f-t)} \right) & t < t_f \\ 0 & t \geq t_f \end{cases} \quad (54)$$

and the equation for η_f now reads

$$n(t_f - t_i)^3 + \frac{6}{\alpha^4} p(\eta_f) = \frac{3}{4\pi v_s^3}. \quad (55)$$

The number density of nucleation sites is found from Eq. (41),

$$\begin{aligned} n_{nuc} \equiv d_{nuc}^{-3} &\simeq n + \frac{p(\eta_f)}{\alpha} - \frac{4\pi v_s^3 p(\eta_f)^2}{\alpha^5} \\ &- \frac{4\pi v_s^3}{3} \frac{p(\eta_f)}{\alpha^4} n \left[z^3 - 3z^2 + 6z - 6 \right] \end{aligned} \quad (56)$$

where $z = \alpha(t_f - t_i)$. Terms like $\exp(-\alpha(t_f - t_c))$ have been neglected. We can write the time difference $t_f - t_i$ as

$$t_f - t_i = (1 - \xi)(t_f - t_c), \quad (57)$$

where $0 \leq \xi < 1$.

Eq. (56) can be simplified by introducing Eq. (55) and keeping only the term z^3 in the parenthesis. Since $\alpha(t_f - t_c) \sim 600$ and we demand $z^3 > 10(3z^2 - 6z + 6)$ then we must have $\xi \leq 0.95$. This is no serious limitation, as we will see. And we hereby decouple the heterogeneous and homogeneous contributions to the number density of nucleation sites. Eq. (56) now reads

$$d_{nuc}^{-3} \simeq n + 4\pi v_s^3 \frac{p(\eta_f)^2}{\alpha^5} \simeq n + \frac{\alpha^3}{16\pi v_s^3}. \quad (58)$$

In the limits of vanishing and huge n , we recover the expected results, $d_{nuc} = d_{nuc,hom}$ (Eq. (50)) and $d_{nuc} = n^{-1/3}$, respectively.

Because of the steepness of the homogeneous nucleation rate all nucleations take place within a 3% interval in η , just below η_f . This means that either homogeneous *or* heterogeneous nucleation determines the mean nucleation distance. Only in a *very* narrow range are there significant contributions from both.

In Figure 5 we have plotted d_{nuc} versus n for fixed bag constant and different s quark masses, in the most optimistic case where $\xi \ll 1$. Notice the step function behavior and the broad range, more than two orders of magnitude, of impurity number densities, resulting in mean nucleation distances above one meter. The largest mean nucleation distance for given parameters is found when $\eta_f \simeq \eta_{f,hom}$. This is a scenario where the shock waves from the nucleated hadron bubbles around the impurities have reheated the whole Universe just before homogeneous nucleation becomes important. The corresponding n can be found from Eq. (55) by neglecting the homogeneous term,

$$d_{nuc,max} = n^{-1/3} \simeq 6(1 - \xi) \left(\frac{\eta_f}{3 \times 10^{-4}} \right) \left(\frac{100\text{MeV}}{T_c} \right)^2 \text{ m}. \quad (59)$$

The corresponding maximal value of l , comoving at $T = 100\text{MeV}$, is found by combining Equations (59) and (1) into

$$l_{max} \simeq 5(1 - \xi) \left(\frac{\eta_f}{3 \times 10^{-4}} \right) \left(\frac{100\text{MeV}}{T_c} \right) \text{ m}. \quad (60)$$

If $\xi < 1/2$ and with a typical value of $\eta_f \simeq 3 \times 10^{-4}$ (for $L \simeq 4B$; otherwise $\eta_f \propto 1/L$) one can have significant nucleosynthesis effects (l of some meters) from impurities for a broad range of n . For $\xi \rightarrow 1$ the approximations used in the derivations above break down, but in this regime the presence of impurities do not lead to large nucleation distances anyway.

The surface tension rises steeply with increasing quark mass for small masses. For realistic u and d quark masses [23] $m_u = 5\text{MeV}$ and $m_d = 10\text{MeV}$ the surface tension increases with about 30% when the s quark contribution is near its maximum. And $d_{nuc,max}$ increases almost 70% to about 11 meters. If we artificially double the surface tension to mimic eventual hadron contributions, we gain more than a factor of 3 on the maximum mean nucleation distance.

IV. CONCLUSION

We have calculated the mean nucleation distance in a homogeneous nucleation scenario where a curvature term contributes to the surface effects. The framework of the multiple

reflection expansion of the MIT bag model has been used to calculate the surface tension and curvature term self-consistently. Inclusion of a curvature term reduces d_{nuc} by about a factor of 7 to less than 2cm.

Furthermore, we have shown that the presence of impurities, for a broad range of densities, can result in mean nucleation distances above one meter. Such large distances are needed if baryon diffusion should not have smeared out generated baryon inhomogeneities before the epoch of nucleosynthesis. It must be emphasized that this conclusion is qualitatively independent of the model used to describe surface effects. We have only assumed that impurities are present, that they lower the energy barrier and that the reheating mechanism is the same regardless of how the hadron bubbles nucleated. Thus, similar effects could be important in other first order transitions as well (see e.g. Ref. [9]).

Unfortunately there are no reliable theoretical expectations for the nature or density of impurities, but we note again the coincidence, that the horizon distance at the electroweak phase transition has expanded to the interesting range of a few meters at the quark-hadron transition.

Eq. (47) for η_f in the homogeneous nucleation scenario tells us how uncertainties in the different parameters influence d_{nuc} , which depends linearly on η_f . We believe the curvature coefficient is well-known, because the major contributions come from gluons and the two massless or very light quarks. A significant surface tension contribution from the pions would raise η_f and thus result in a larger $d_{nuc,max}$ and an even broader interval of impurity number densities, where the mean nucleation distances is above one meter.

We have throughout used the self-consistently calculated latent heat of $4B$, even though some recent lattice calculations [8] suggest that the latent heat is about ten times smaller. A temperature dependent bag constant that increases with increasing temperature may reproduce such a result, but no theoretical predictions of such a temperature dependence exist. However, η_f , d_{nuc} , and l are all inversely proportional to the latent heat. Thus, a tenfold decrease in L results in a tenfold increase in η_f , d_{nuc} , and l .

In Ref. [20] the spectrum of nucleation site separations is calculated. A duality between the nucleation sites and large baryon concentration sites is assumed and the effect on nucleosynthesis calculated. If impurities play a major role, the nucleation site spectrum would look different. For randomly distributed impurities the spectrum would be broad. A sort of regularity in the impurity distribution would result in a very narrow distribution around the mean nucleation distance. Such an approximation is often used in actual inhomogeneous nucleosynthesis calculations.

A serious problem with the bag model in the form used in this paper is the local minimum in the free energy at about 10 fm, even above the critical temperature [13]. One might think about removing it by introducing further corrections in the density of states related to zero point energy, color singlet restrictions, etcetera, but no recipe exists at the moment. We note however, that such effects will be most important for small radii, and since the maximum of the free energy barrier typically lies beyond a radius of 50 fm in the results presented above, the conclusions of the present investigation are not likely to be affected much.

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FIGURES

FIG. 1. The latent heat as a function of the s quark mass for $B^{1/4} = 145\text{MeV}$. The uppermost curve includes only pions, whereas the other curves from above include mesons up to masses of 547MeV, 892MeV and 1020MeV, respectively.

FIG. 2. The free energy as function of bubble radius for different temperatures in MeV at $B^{1/4} = 145\text{MeV}$ and $m_s = 150\text{MeV}$, with curvature. The critical temperature gives the solid curve. The dashed curve is for the maximum supercooling, η_f , where almost all hadron bubbles are nucleated with a radius, $R_+ \simeq 55\text{fm}$. The dotted curve is still for η_f but with $\gamma = 0$. The dash-dotted curve corresponds to an even larger supercooling where the local minimum at $R_- \simeq 10\text{fm}$ can no longer be ignored.

FIG. 3. The maximum supercooling, η_f , versus m_s . Solid curves are for $B^{1/4} = 145\text{MeV}$, the upper for $\gamma = 0$. Dashed curves are for $B^{1/4} = 245\text{MeV}$, the upper for $\gamma = 0$. The dotted curves correspond to the approximation in Eq. (47).

FIG. 4. The mean nucleation distance as a function of the s quark mass. The solid curves are for $B^{1/4} = 145\text{MeV}$, the uppermost for $\gamma = 0$. The dotted curves for $B^{1/4} = 245\text{MeV}$. Dashed curves are the corresponding approximative expressions in Eqs. (2) and (3).

FIG. 5. The mean nucleation distance as a function of the impurity number density for different s quark masses at $B^{1/4} = 145\text{MeV}$. From left to right the masses are 100MeV, 150MeV and 200MeV, respectively.









